Journal of Groundwater Research, Vol.8-9/1, December 2019/2020

Analytical Solutions of Advection-Dispersion Equation with Variable Coefficients and their Correctness

Naveen Kumar
Professor (Retired) of Mathematics, Institute of Science, Banaras Hindu University, Varanasi-221005
Email: navkumar50s@gmail.com

Abstract

This study outlines analytical solutions, obtained a decade earlier, for temporal/spatial solute dispersion in unsteady/linearly spatially dependent flow through a semi-infinite domain, and discusses their correctness.

Keywords: ADE, Analytical Solutions, Correctness

1. Introduction

The advection-dispersion equation (ADE) describes solute transport with position and time along or against laminar flow in an open medium or Darcy flow through a porous medium. ADE may be derived using the law of conservation of mass and Fick's first and second laws. In a still medium the solute transport is governed by simply the diffusion equation. Both are partial differential equations (PDEs) of second order. These equations are of parabolic type, their closed form analytical solution or numerical solution may be obtained using a first or solution type initial condition in time and two boundary conditions. A homogeneous initial condition refers to an initially solute-free domain. In a semi-infinite or finite medium, the first boundary condition is usually assumed at the origin of the medium, and one such non-homogeneous condition refers to the concentration of the source of the solute mass to be dispersed. This non-homogeneous condition may be any of the three types of condition. A first or solution type condition defines a uniform source, whereas a third or mixed type condition defines a source having concentration either increasing or decreasing with time. The source may occur at a point other than the origin but in that case the origin needs to be shifted to that point through a coordinate transformation, as the solution of an ODE (Ordinary Differential Equation) or a PDE is obtained for convenience, in the neighborhood of the origin. Further, the other governing equations also need to be transformed through this transformation. The continuous time domain of the source may comprise of piecewise continuous domains with different source concentration in each time zone. The second boundary condition may be assumed according to the dispersion problem.

In an infinite domain, as the origin is difficult to define, the source concentration may be defined through a non-homogeneous term of the ADE in the form of Dirac delta function. And this is the correct way which Sanskrityayn and Kumar (2018) have demonstrated. They found a major flaw in defining it at the origin, $x = 0$ through an initial condition in the domain $x < 0$ in the form of a Heaviside function, as in Selvadurai (2004, 2008) and Hayek (2017). It is an important observation and should be taken care of. Seldom open or porous media, including all naturally occurring aquifers and oil reservoirs, are homogeneous. Through such a heterogeneous medium, transport properties vary with position/time, and the solute transport through such medium may be described by an ADE with temporally/spatially dependent coefficients, instead of through an ADE with constant coefficients. To get an analytical solution of an ADE, an integral transform technique like LITT (Laplace integral transform technique) is best suited, as it reduces the dispersion governing equations into a second order ODE along with two boundary conditions in the Laplacian domain. A Hankel integral transform technique reduces the dispersion problem into an initial value problem of first order but this technique may be used effectively in cylindrical coordinate system only.

To get an analytical solution of the ADE with variable coefficients has been a difficult task using these techniques except in few cases in which the variable coefficients have simple forms. Barry and Sposito (1989) concluded that closed form analytical solutions of the ADE with temporally dependent coefficients were not possible in a semi-infinite medium where the dispersion coefficient (*D*) did not follow the dispersion rule $D \propto u^n$, $1 \le n \le 2$ (Freeze and Cherry, 1979), *u* is the advective velocity. However, analytical solutions are feasible in case the dispersion rule is followed for an integral value $n =$ 1 or 2. Large number of references related with a heterogeneous medium and solute transport through it may be obtained from Sanskrityayn et al. (2016, 2017, 2018a,b), in which analytical solutions of the ADE with a sufficient number of temporally and spatially dependent coefficients have been obtained in infinite media using Green's Function Method (GFM). The solute transport is said to occur in Euclidean framework for integer values of the index that is for $n =$ 1 or 2, in the dispersion rule, but for any permissible real value like $n =$ 1.5 or 1.75, it is said to be in fractal framework (Wheatcraft and Tyler, 1988).

Recently ADE has been solved analytically in the fractal framework too but in a finite domain only, using EFSM (Extended Fourier Series Method) by Bharati et al. (2015, 2017, 2018, 2019), in which a new SLP (Sturm Liouville's Problem) has paved the way for the solution in the form of extended Fourier series converging to the desired solution with only first five terms. Also, one such solution is in very good agreement with the already existing numerical solution of the same dispersion problem. This convergence had been the issue in the previous works using the same method but with a different name GITT (Generalized Integral Transform Technique), which occurred for terms varying from thirty to a few hundred, depending upon the nature of the problem. As a result it did not yield the analytical solution. A lot of works using GITT are cited in Bharati et al. (2015, 2017, 2018, 2019).

The objective of the present study is to appraise the analytical solutions, obtained a decade earlier, of the ADE with temporally dependent or spatially dependent or temporally-spatially dependent coefficients in finite and semi-infinite, and the efforts to show these solutions wrong in the light of already drawn conclusion by Barry and Sposito (1989). But the issues raised in these have been well defended. The outcome of these discussions is that though such analytical solutions are not exact, each has negligible error. A new transformation paved the way to get these analytical solutions. The transformation reduced the ADEs with variable coefficients, for which their analytical solutions did not exist, into an ADE with constant coefficients. These works, alongwith the transformations used are listed in section 3. Also, the discussion which was reported in context of the correctness of these solutions is briefly stated.

2. New Transformation

If the dispersion coefficient D is directly proportional to the advective unsteady velocity u, then in one-dimension, the advection-dispersion equation (ADE) may be written as

$$\frac{\partial C}{\partial t} = D_0 f(mt)\frac{\partial^2 C}{\partial x^2} - u_0 f(mt)\frac{\partial C}{\partial x}, \tag{1}$$

where m is an unsteady parameter and D_0 and u_0 are the constant dispersion coefficient and velocity, respectively. To get rid of the temporal dependent coefficients of the ADE in Eq. (1), the Kirchhoff transformation (Crank, 1975)

$$T = \int f(mt)dt, \tag{2}$$

may be used. Eq. (2) introduces a new time variable, from which we may have

$$\frac{dT}{dt} = f(mt), \tag{3}$$

so $$\frac{\partial C}{\partial t} = \frac{\partial C}{\partial T}\frac{dT}{dt} = f(mt)\frac{\partial C}{\partial T},$$

and the ADE in Eq. (1) reduces into an ADE with constant coefficients in the (x,T) domain as

$$\frac{\partial C}{\partial T}=D_0\frac{\partial^2 C}{\partial x^2}-u_0\frac{\partial C}{\partial x}. \tag{4}$$

Eq. (3) may be written as

$$\frac{dT}{f(mt)}=\frac{dt}{1} \tag{5}$$

It may be assumed to be part of a system of three ordinary differential equations (ODEs)

$$\frac{dT}{f(mt)}=\frac{dt}{1}=\frac{d\phi}{f_1(t,T,\phi)}, \tag{6}$$

Let it be the auxiliary system of a linear first order partial differential equation (PDE) in terms of a dependent variable ϕ as follows (see the theorem on first order linear PDE in Appendix)

$$f(mt)\frac{\partial\phi}{\partial T}+\frac{\partial\phi}{\partial t}=f_1(t,T,\phi). \tag{7}$$

Now let us consider an ADE with spatio-temporal coefficients as

$$\left[\frac{\partial}{\partial t}-\frac{\partial}{\partial x}\left(D_0 f_1(x,t)\frac{\partial}{\partial x}-u_0 f_2(x,t)\right)\right]C=0, \tag{8}$$

and

$$\frac{\partial}{\partial X}=f_1(x,t)\frac{\partial}{\partial x}-f_2(x,t). \tag{9}$$

Applying the latter to a solution $\varphi(x,X)$, we have a linear first order partial differential equation

$$f_1(x,t)\frac{\partial\varphi}{\partial x}-\frac{\partial\varphi}{\partial X}=f_2(x,t)\varphi. \tag{10}$$

Its auxiliary system of three ODEs may be written as

$$\frac{dx}{f_1(x,t)}=\frac{dX}{-1}=\frac{d\phi}{f_2(x,X)\phi}, \tag{11}$$

from which we have one ODE as

$$\frac{dX}{dx}=-\frac{1}{f_1(x,t)}, \tag{12}$$

whose solution may be written as

$$X=-\int\frac{dx}{f_1(x,t)}. \tag{13}$$

Eq. (12) may be used as a transformation, which is new, to introduce a new space variable *X*. The percipience of this transformation may also be carried out as an extension of Eq. (2). The expression for X may be obtained from Eq. (13), *e.g.* for $f_1(x,t)=f(mt)$ we have

$$X=-\frac{x}{f(mt)}. \tag{14}$$

Using Eq. (12), we have

$$\frac{\partial}{\partial x}=\frac{\partial}{\partial X}\frac{dX}{dx}=-\frac{1}{f_1(x,t)}\frac{\partial}{\partial X},$$

and the ADE in Eq. (8) may be written as

$$\frac{\partial C}{\partial t}=-\frac{1}{f_1(x,t)}\frac{\partial}{\partial X}\left[-D_0\frac{\partial}{\partial X}-u_0 f_2(x,t)\right]C. \tag{15}$$

Thus, for suitable expressions of $f_1(x,t)$ and $f_2(x,t)$, the ADE in Eq. (8) may be reduced into an ADE with constant coefficients, whose analytical solutions subject to a variety of initial and boundary conditions are already known. Thus, analytical solutions of the ADE with spatial/temporal coefficient(s), in some naturally occurring and theoretically established forms related with groundwater velocity and dispersion of solute through it, may be obtained in terms of known closed form functions. In some of the works done a decade earlier, stated in the next section, using different combinations of both the variable coefficients and a series of transformations, including the two foremost transformations as in Eq. (2) and Eq. (12), the respective ADEs, have been reduced to an ADE with constant coefficients in terms of a set of new independent variables (Z,T), as

$$\frac{\partial C}{\partial T}=D_0\frac{\partial^2 C}{\partial Z^2}-u_0\frac{\partial C}{\partial Z}, \qquad (16)$$

where Z is another space variable introduced through a separate coordinate transformation in terms of X. The analytical solutions of the ADE in the form as in Eq. (16), subject to a variety of initial and two boundary conditions, are known, obtained much earlier by using Laplace Integral Transformation Technique (LITT), and are compiled in many works like that of van Genutchen and Alves (1982).

3. Analytical Solutions for temporal/spatial dispersion and their correctness

A variety of hydro-geologically suited expressions for $f_1(x,t)$ and $f_2(x,t)$ have been chosen and the analytical solutions of the ADEs with such coefficients have been obtained. The transformations used do not change the nature of initial and boundary conditions prescribed in the (x,t) domain; a finite domain remains finite, a semi-infinite domain remains the same, and at $t=0$, one gets $T=0$. These combinations along with the works in which they have been used, are listed as follows:

I	$f_1(x,t)=f(mt)$	and	$f_2(x,t)=1$
II	$f_1(x,t)=(1+ax)^2$	and	$f_2(x,t)=(1+ax)$
III	$f_1(x,t)=f(mt)(1+ax)^2$	and	$f_2(x,t)=f(mt)(1+ax)$,
IV	$f_1(x,t)=f^2(mt)(1+ax)^2$	and	$f_2(x,t)=f(mt)(1+ax)$, and
V	$f_1(x,t)=f_2(mt)(1+ax)^2$	and	$f_2(x,t)=f_1(mt)(1+ax)$,

The linear non-homogeneous spatial velocity has been considered, based on the theoretical and experimental results established by Serrano (1992), where a is the heterogeneity parameter such that ax is dimensionless and its values may not occur beyond 0.5. Exponentially decelerating and exponentially accelerating expressions along with some more increasing and decreasing functions have been considered for $f(mt)$ such that for $m=0$, $f(mt)=1$.

ADEs with the two sets of combinations in I & II have been solved in two different sections in a finite domain, using uniform and varying continuous sources, respectively, by Kumar et al., (2009); using a pulse uniform source in a semi-infinite medium by Jaiswal et al., (2009); and for a continuous uniform source in a semi-infinite medium by Kumar et al. (2010). The III combination has also been considered in a separate section of Kumar et al. (2010). With the combination I, the ADE with variable coefficients is reduced to an ADE with constant coefficients as in Eq. (16), where the new independent variables have the expressions

$$X=-\int\frac{dx}{f(mt)}=-\frac{x}{f(mt)},\qquad Z=-X,\qquad \text{and}\qquad T=\int\frac{dt}{f(mt)}.$$

With the combination in II, Eq. (16) is obtained using the expressions

$$X=-\int\frac{dx}{(1+ax)^2}=\frac{1}{a(1+ax)},\qquad Z=-\ln(aX),\qquad \text{and}\qquad T=t,$$

and with the combination in III, Eq. (16) is obtained using the same transformations for X and Z as with the combination in II with an additional transformation for T, that is, by using the expressions

$$X=\frac{1}{a(1+ax)},\qquad Z=-\ln(aX)\qquad \text{and}\qquad T=\int\frac{dt}{f(mt)}.$$

In Kumar et al. (2012), the combination IV is chosen for a continuous uniform source in a semi-infinite medium. The ADE with this combination of variable coefficients is reduced to Eq. (16), using the expressions for new independent variables

$$T^* = \int f(mt)dt, \; X = \frac{1}{a}\ln(1+ax), \qquad Z = \frac{f_0(mt)}{f(mt)}X, \qquad f_0(mt) = 1-(aD_0/u_0)f(mt), \quad \text{and}$$

$$T = \int f_0^2(mt)dt.$$

The last combination V has been chosen in Yadav et al. (2011) and Singh et al. (2012). A pulse uniform source in the former work and a pulse varying source in the latter are considered in a semi-infinite medium. The ADE with variable coefficients is reduced to an ADE as in Eq. (16), using the expressions:

$$T^* = \int f_1(mt)dt, \; X = \frac{1}{a}\ln(1+ax), \; Z = \frac{f_1(mt)f_3(mt)}{f_2(mt)}X, \; f_3(mt) = 1-a\frac{D_0 f_2(mt)}{u_0 f_1(mt)},$$

$$T = \int \frac{f_1^2(mt)f_3^2(mt)}{f_2(mt)}dt.$$

In both the papers a combination of two temporal functions is taken as $f_1(mt) = \exp(mt)$ and $f_2(mt) = \exp(-mt)$. Both may be interchanged without any difficulty. Any other combination of the two temporal functions may also be tried out. Some of the above dispersion problems have been extended in two-dimensional horizontal plane by Jaiswal et al. (2011) and Yadav et al. (2012).

The salient features of these analytical solutions are as follows:

(i) The transformations, as stated above too, do not change the nature of initial and boundary conditions prescribed in the (x,t) domain; a finite domain remains finite, a semi-infinite domain remains the same, and at $t=0$, one gets $T=0$.

(ii) For $m=0$, $f(mt)=1$. Thus, for $a=0/m=0$, in each work cited above, the ADE with temporal/spatial coefficients reduces to the ADE with constant coefficients in the (x,t) domain, and the respective solution reduces to that of the ADE with constant coefficients.

(iii) In each paper, in which $f(mt)$ occurs, the analytical solutions are illustrated for the decelerating function $f(mt)=\exp(-mt)$ and accelerating function(s) $f(mt)=\exp(mt)$ / $(1-mt)^{-1}$ and are compared with the particular solution obtained for $f(mt)=1$. The solution of the ADE with temporal coefficient(s) not only exhibits very closely the same concentration pattern as that of the ADE with constant coefficient but the concentration pattern shows the expected pattern according to the behavior of the temporally dependent dispersion. The dispersion with the expression $D_0\exp(-mt)$ will be less, while that with $D_0\exp(mt)$ will be higher than that with D_0, and the difference in the concentration values at a particular position and time between the three solutions occurs accordingly.

(iv) Similarly, analytical solutions of the ADE with spatial coefficients also show the expected solute transport pattern.

Deng and Qui (2012) tried to prove the solution in Eq. (35) of Kumar et al. (2010) and the other solutions derived in the related works cited above to be wrong. Their assertion seems to have a firm belief on the conclusion derived by Barry and Sposito (1989) that closed form analytical solution of ADE with temporal coefficient(s) in a semi-infinite medium is not possible. They are based on that Eq. (14) has been used as a transformation. Once others (*e.g.*, Hayek, 2017) started reporting the observations of Deng and Qui (2012), it became imperative to clarify it. It was made distinctively clear in Sanskrityayn and Kumar (2018) that Eq. (12) is the transformation used, not Eq. (14), to get the solution in Eq. (35) of Kumar et al. (2010). For example, Eq. (2) is the transformation used to reduce the ADE in Eq. (1) to another ADE in Eq. (4) but an expression for T, obtained from Eq. (2) for an expression of $f(mt)$, is not the transformation. Similarly, Eq. (14) obtained from Eq. (12) for $f_1(x,t) = f(mt)$ is not that transformation but only provides the expression for the new space variable X. Also, it was shown that the transformations introduced and used in these works are correct. But the mathematical discussion carried out in Deng and Qui (2012) was fruitful and laid the foundation for developing pertinent transformations getting relevant analytical solutions of the ADE with a variety of spatio-temporal coefficients in infinite media by Sanskrityayn et al. (2016, 2017, 2018a,b).

Deng et al. (2019) tried afresh to prove the said solutions to be wrong on the basis of three points: (i) the derivative in Eq. (12) which is also Eq. (7) of Sanskrityayn and Kumar (2018), should be partial derivative; (ii) the solution in Eq. (35) of Kumar et al. (2010) does not satisfy the related ADE, and (iii) the variable coefficients of the ADE considered cannot be used for arbitrary functions. All the three issues are clarified in Jaiswal et al. (2020). Regarding the first issue it is clear that the derivative in Eq. (12) cannot be a partial derivative. Also, although an analytical solution of ADE with constant coefficients subject to a certain set of initial and boundary conditions obtained by using LITT satisfies the ADE, hence it is an exact solution yet that of ADE with variable coefficient(s) may not be exact, one such solution may be an approximate solution but the error of approximation due to the remainder of terms should be negligible as is the case with the solution in Eq. (35) of Kumar et al. (2010). It is demonstrated through a Table drawn in Jaiswal et al. (2020). This table contains the concentration values evaluated from the solution in Eq. (35) of Kumar et al. (2010) for $f(mt) = \exp(-mt)$, $f(mt) = \exp(mt)$ and $f(mt) = 1$, at two values of time, along with the respective value of the error term. Regarding the exponentially accelerating expression $f(mt) = \exp(mt)$ chosen, its limitation is already explained in Kumar et al. (2010) and Yadav et al. (2011). This expression may only be used for small values of time in case of uniform continuous source, particularly in real hydro-geological conditions. For a varying source, it may be viewed from figures drawn in Yadav et al. (2011) and other works that for this exponentially accelerating function the input concentration increases with the decelerating rate approaching to the saturation fast. So there is no effect of the source on the polluted domain, once a saturation stage is reached. The work of Gharehbaghi (2016) is worth mentioning here regarding such comparison, in which the solutions of the ADE with time-dependent coefficient(s) in semi-infinite media obtained by using a novel numerical model based on the finite volume method are validated through the analytical solution in Eq. (35) of Kumar et al. (2010).

Thus, analytical solutions obtained in the cited papers are correct though they may be approximate solutions but have negligible error. In fact, there is no necessity of writing Eq. (9) or Eq. (10). Transformation in Eq. (12) or Eq. (13) may be written directly as Eq. (2). Eq. (9) is written to have the coefficients of the ADE in Eq. (8). It guided to write a transformation in Eq. (12) to get rid of the variable coefficients from the space derivative terms of the ADE. These were not possible till then. To get some other transformation like in Eq. (2) or Eq. (12) to eliminate the coefficient of the time derivative term or more coefficients of the ADE, an equation similar to Eq. (9) or an extended equation may be written. For example, we may have

$$\frac{\partial}{\partial X} = f_1(x,t)\frac{\partial}{\partial x} - f_2(x,t)\frac{\partial}{\partial t} + f_3(x,t), \tag{17}$$

or some other equation like

$$\frac{\partial}{\partial T} = f_1(x,t)\frac{\partial}{\partial x} + f_2(x,t)\frac{\partial}{\partial t} - f_3(x,t). \tag{18}$$

Each will be equivalent to the system of six ODEs, from where a suitable transformation may be developed. If a transformation between old and new space variables is only required, it is sufficient to have Eq. (9) or Eq. (10). Such transformation may also be extracted in other coordinate systems like polar, spherical, and cylindrical coordinate systems. But in their closure, Deng et al. (2020) still maintained that in Eq. (12), the derivative should be partial, Eq. (14) has been used as a transformation to get the solution in Eq. (35) of Kumar et al. (2010), and due to the presence of variable t, Eq. (10) is an ill-posed problem. The last one is the new reason, along with some more fictitious issues raised obstinately to prove their point. But as discussed in this paragraph it is clear that neither Eq. (9) nor Eq. (10) is an ill-posed problem. Still treating t as the third independent variable we need to write an extended equation like the one in Eq. (17) but Eq. (12) will be there in the auxiliary system of the PDE formed by this equation.

4. Conclusion

The conclusion was drawn in 1989 that the analytical solution of advection dispersion equation with time dependent transport parameters in semi-infinite medium is not possible. Two decades later analytical solutions of such ADEs with different sets of variable coefficients were published. But questions were raised time and again about the correctness of these solutions. These discussions in research are not impertinent at all, and must be welcomed. They provide new insights and way to get into the new domain of thoughts.

Acknowledgement

The author is extremely grateful to the reviewers for their valuable comments and minute observation.

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Appendix

A linear first order PDE for $z = f(x, y)$ may be written in general form as

$$f_1(x,y)\frac{\partial z}{\partial x} + f_2(x,y)\frac{\partial z}{\partial y} = f_3(x,y)z + f_4(x,y) \qquad \text{(A1)}$$

A quasi-linear first order PDE has a general form

$$f_1(x,y,z)\frac{\partial z}{\partial x} + f_2(x,y,z)\frac{\partial z}{\partial y} = f_3(x,y,z) \qquad \text{(A2)}$$

A first order linear PDE is equivalent to Lagrange system of three first order ordinary differential equations (ODEs). So PDE in Eq. (A2) is equivalent to:

$$\frac{dx}{f_1(x,y,z)} = \frac{dy}{f_2(x,y,z)} = \frac{dz}{f_3(x,y,z)}, \qquad \text{(A3)}$$

or $$\frac{dx}{dy} = \frac{f_1(x,y,z)}{f_2(x,y,z)} \quad \text{or} \quad \frac{dy}{dx} = \frac{f_2(x,y,z)}{f_1(x,y,z)}, \qquad \text{(A4)}$$

and similar two other ODEs. Any two independent solutions of the set of three solutions obtained by integrating each ODE, $u_1(x,y,z) = c_1$ and $u_2(x,y,z) = c_2$, forms the solution of the given first order linear PDE as $F(u_1, u_2) = 0$, where c_1 and c_2 are arbitrary constants and F is an arbitrary function. This theorem with proof may be found in the initial chapters of any good book on partial differential equation.

Corresponding Author

Naveen Kumar

Professor (Retired) of Mathematics, Institute of Science, Banaras Hindu University, Varanasi-221005

(Mailing address: 2A/T10-801, Mandakini, Avadh Vihar, P.O. Barauna, Lucknow-226002)

Email: navkumar50s@gmail.com

Manuscript History

Received on May27,2020; Revised on June,2020; Accepted on Sept.14, 2021